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2NP8



Structural Basis for the Inhibition of Aurora A Kinase by High Affinity Disubstituted Pyrimidine Inhibitors

Characteristics

Release Date: 26-Dec-2006 Exp. Resolution: 2.25 Å

Classification Compound

Transferase
 Molecule: Serine/threonine-protein
 Polymer: 1 Type: polypeptide
 Chains: A, B
 EC#: 2.7.11.1

Authors

Tari, L.W., Hoffman, I.D., B.M.J., Nix, J., Nelson, K.J., Swanson, R.V.

3CON



Crystal structure of Aurora-A in complex with a peptide inhibitor

Characteristics

Release Date: 17-Feb-2009 Exp. Resolution: 2.70 Å

Classification Compound

Transferase
 Molecule: Serine/threonine-protein
 Polymer: 1 Type: polypeptide
 Chains: A, B
 EC#: 2.7.11.1
 Fragment: kinase domain (UNP residues 124-400)
 Mutation: K124A, Q154N, A203S, E336D

Authors

Wiesmann, C., Raswason, T.E.

2VGP



CRYSTAL STRUCTURE OF AURORA B KINASE IN COMPLEX WITH AN AMINOTHIAZOLE INHIBITOR

Characteristics

Release Date: 26-Feb-2008 Exp. Resolution: 1.70 Å

Classification Compound

Transferase
 Molecule: SERINE/THREONINE-PROTEIN KINASE
 Polymer: 1 Type: polypeptide
 Chains: A, B
 EC#: 2.7.11.1
 Fragment: RESIDUES 78-361
 Molecule: INNER CENTROMERE PROTEIN
 Polymer: 2 Type: polypeptide
 Chains: C, D
 Fragment: RESIDUES 798-840



Authors Andersen, C.B. , Wan, Y. , Ch
Liu, Y. , Sessa, F. , Villa, F. ,
Musacchio, A. , Gray, N.S.

Crystal structure of mouse Aurora A (Asn186->Gly
> Leu) in complex with 1-{5-[2-(1-methyl-1H-pyrro
lylamino)-ethyl]-thiazol-2-yl}-3-{3-(trifluoromethyl

Characteristics Release Date: 12-May-2009 Exp. I
Resolution: 2.90 Å
Classification Transferase
Compound Molecule: serine/threonine kinase
Polymer: 1 Type: polypeptide
Chains: A
EC#: 2.7.11.1
Fragment: Aurora A kinase domain
Mutation: N186G, K240R, M302L

Authors Oslob, J.D. , Yu, C. , Romano



Crystal structure of mouse Aurora A (Asn186->Gly
> Leu) in complex with [7-(2-{2-[3-(3-chloro-phen
yl)-ethylamino]-pyrazolo[4,3-d]pyrimidin-1-yl]-a

Characteristics Release Date: 12-May-2009 Exp. I
Resolution: 2.50 Å
Classification Transferase
Compound Molecule: serine/threonine kinase
Polymer: 1 Type: polypeptide
Chains: A
EC#: 2.7.11.1
Fragment: Aurora A kinase domain
Mutation: N186G, K240R, M302L

Authors Elling, R.A. , Oslob, J.D. , Yu,
M.J.



STRUCTURE OF AURORA B KINASE IN COMPLEX W

Characteristics Release Date: 01-Jul-2008 Exp. M
Resolution: 1.85 Å
Classification Cell Cycle/transferase
Compound Molecule: SERINE/THREONINE-PR
Polymer: 1 Type: polypeptide
Chains: A, B
EC#: 2.7.11.1
Fragment: CATALYTIC KINASE DOM
Molecule: INNER CENTROMERE PF
Polymer: 2 Type: polypeptide
Chains: C, D
Fragment: RESIDUES 798-840
Authors Girdler, F. , Sessa, F. , Paler
Ridgway, E. , Musacchio, A. ,



CRYSTAL STRUCTURE OF AURORA B KINASE IN COMPLEX
WITH REVERSINE INHIBITOR

Characteristics Release Date: 28-Oct-2008 Exp. M
Resolution: 1.70 Å
Classification Transferase
Compound Molecule: SERINE/THREONINE-PR
Polymer: 1 Type: polypeptide
Chains: A, B
EC#: 2.7.11.1



Fragment: RESIDUES 78-361

Molecule: INNER CENTROMERE PF
 Polymer: 2 Type: polypeptide
 Chains: C, D
 Fragment: RESIDUES 797-840

Authors

D'Alise, A.M. , Amabile, G. ,
 Giorgio, F.P. , Bartiromo, M. ,
 F. , Musacchio, A. , Cortese,

☒ **2WEV****TRUNCATION AND OPTIMISATION OF PEPTIDE IN CYCLIN A THROUGH STRUCTURE GUIDED DESIGN****Characteristics**

Release Date: 09-Jun-2009 Exp. A
 Resolution: 2.30 Å

Classification Compound**Transferase**

Molecule: CELL DIVISION PRO
 Polymer: 1 Type: polypep
 Chains: A, C
 EC#: 2.7.1.37
 Other Details: TRIAZOL-1-METHYL-

Molecule: CYCLIN-A2
 Polymer: 2 Type: polypep
 Chains: B, D
 Fragment: RESIDUES 173-432
 Other Details: CAP-TETRAPEPTIDE

Molecule: ARG-ARG-B3L-MEA
 Polymer: 3 Type: polypep
 Chains: E, F

Authors

Kontopidis, G. , Andrews, M.J.
 Plater, A. , Innes, L. , Renac
 A. , Fischer, P.M.

☒ **2WFY****TRUNCATION AND OPTIMISATION OF PEPTIDE IN CYCLIN A THROUGH STRUCTURE GUIDED DESIGN****Characteristics**

Release Date: 09-Jun-2009 Exp. A
 Resolution: 2.53 Å

Classification Compound**Transferase**

Molecule: CELL DIVISION PROTEIN
 Polymer: 1 Type: polypeptide
 Chains: A, C
 EC#: 2.7.1.37

Molecule: CYCLIN-A2
 Polymer: 2 Type: polypeptide
 Chains: B, D
 Fragment: RESIDUES 173-432

Molecule: ARG-ARG-B3L-PHE
 Polymer: 3 Type: polypeptide
 Chains: E, F

Authors

Kontopidis, G. , Andrews, M.J.
 Plater, A. , Innes, L. , Renac
 A. , Fischer, P.M.

☒ **2WHB****TRUNCATION AND OPTIMISATION OF PEPTIDE IN CYCLIN A THROUGH STRUCTURE GUIDED DESIGN****Characteristics**

Release Date: 09-Jun-2009 Exp. A
 Resolution: 2.90 Å

Classification Compound**Transferase**

Molecule: CELL DIVISION PRO
 Polymer: 1 Type: polypep

**Authors**

Chains: A, C
EC#: 2.7.1.37
Other Details: TRIAZOL-1-METHYL-
Molecule: CYCLIN-A2
Polymer: 2 Type: polypep
Chains: B, D
Fragment: RESIDUES 173-432
Molecule: ARG-ARG-L30-PFF
Polymer: 3 Type: polypep
Chains: E, F
Authors Kontopidis, G. , Andrews, M.J.
Plafer, A. , Innes, L. , Renac
A. , Fischer, P.M.



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